Homework 2, Dowling

1. The provided code creates a data frame called "df1", with 3 columns: Name, State and Sales. There are 12 rows of data in the table.

```
State Sales
      Name
     James
                 Alaska
      Paul California
2
                Texas 31
   Marico North Carolina
4
                          12
  Samantha California
Ravi Texas
5
                          13
    Kavi Texas
Raghu Alaska
Richards —
                          9
8 Richards
                          31
    George North Carolina
                          18
     Ema Alaska 16
11 Samantha
             California 18
12 Catherine
            Texas
```

The following two commands appear to be different ways to sum Sales by State:

The first few rows (head) of WorldCupMatches look like this (not easy to read in larger font size, so I decreased the size):

```
> library(rstudioapi)
 > setwd(dirname(rstudioapi::getActiveDocumentContext()$path))
 > wc <- read.csv("../data/WorldCupMatches.csv")</pre>
> head(wc)

        Year
        Datetime
        Stage
        Stadium
        City Home.Team.Name
        Home.Team.Goals
        Away.Team.Goals

        1 1930 13 Jul 1930 - 15:00
        Group 1
        Pocitos Montevideo
        France
        4
        1

        2 1930 13 Jul 1930 - 15:00
        Group 4
        Parque Central Montevideo
        USA
        3
        0

2 1930 13 041 1930 - 13:00 Group 4 Parque Central Montevideo USA 3
3 1930 14 Jul 1930 - 12:45 Group 2 Parque Central Montevideo Yugoslavia 2
4 1930 14 Jul 1930 - 14:50 Group 3 Pocitos Montevideo Romania 3
5 1930 15 Jul 1930 - 16:00 Group 1 Parque Central Montevideo Argentina 1
6 1930 16 Jul 1930 - 14:45 Group 1 Parque Central Montevideo Chile 3
Away.Team.Name Win.conditions Attendance Half.time.Home.Goals Half.time.Away.Goals
                                                                                                                                               2
3
1
3
                                                                                                                                                                              1
                                                                                                                                                               Referee
                                                                            3 0 LOMBARDI Domingo (URU)
2 0 MACIAS Jose (ARG)
              Mexico
                                                            4444
           Belgium
                                                           18346
                                                                                                 2 1 0 1
             Brazil
                                                         24059
3
                                                                                                                                   0 TEJADA Anibal (URU)
0 WARNKEN Alberto (CHI)
                                                                                                                                   0 REGO Gilberto (BRA)
                                                                                                                                   0 CRISTOPHE Henry (BEL)
                                                               Assistant.2 RoundID MatchID Home.Team.Initials Away.Team.Initials
                                                                                                                                       YUG
```

4	LANGENUS Jean	(BEL)	MATEUCCI Francisco	(URU)	201	1098	ROU	PER
5	SAUCEDO Ulises	(BOL)	RADULESCU Constantin	(ROU)	201	1085	ARG	FRA
6	APHESTEGUY Martin	(URU)	LANGENUS Jean	(BEL)	201	1095	CHI	MEX

a. Rows/cols

> nrow(wc) [1] 852 > ncol(wc) [1] 20

b. Summary

> summary(wc)					
Year	Datetime	Stage	Stadium	City	Home.Team.Name
Min. :1930	Length:852	Length:852	Length:852	Length:852	Length: 852
1st Qu.:1970	Class :character	Class :character	Class :character	Class :character	Class :character
Median :1990	Mode :character	Mode :character	Mode :character	Mode :character	Mode :character
Mean :1985					
3rd Qu.:2002					
Max. :2014					
		3	ration and all the con-	2112	W-16 - 1' W G1-
Home.Team.Goal		-	Win.conditions		Half.time.Home.Goals Min. :0.0000
Min. : 0.000 1st Ou.: 1.000		Length:852 Class:character	Length:852 Class:character		Min. :0.0000 1st Ou.:0.0000
Median : 2.000	-	Mode :character	Mode :character	-	Median :0.0000
		Mode :Character	Mode :Character		Median :0.7089
Mean : 1.811 3rd Qu.: 3.000					3rd Ou.:1.0000
Max. :10.000				-	Max. :6.0000
Max10.000	Max7.000			NA's :2	Max0.0000
Half.time.Away	.Goals Referee	Assistant.1	Assistant.2		
Min. :0.0000		Length:852	Length:852	Min. :	201
1st Ou.:0.0000		-			262
Median :0.0000					337
Mean :0.4284		accel node chai	idetei ilode iellai		661773
3rd Ou.:1.0000				3rd Qu.:	
Max. :5.0000					410600
101000				114111	110000
MatchID	Home.Team.In	itials Away.Team.Ir	nitials		
Min. :	25 Length: 852	Length:852			
1st Qu.: 1	189 Class :chara	cter Class:chara	acter		
Median: 2	191 Mode :chara	cter Mode :chara	acter		
Mean : 61346	868				
3rd Qu.: 43950	059				
Max. :300186	515				

c. Unique locations

> length(unique(wc\$City))
[1] 151

d. Average attendance

> mean(wc\$Attendance, na.rm = TRUE)
[1] 45164.8

e. Total goals per team

f. Average annual attendees

- > attend <- aggregate(wc\$Attendance, by=list(wc\$Year), FUN=mean, na.rm = TRUE)
- > colnames(attend) <- c("Year", "AverageAttendance")</pre>
- > print(head(attend))

Year AverageAttendance
1 1930 32808.28
2 1934 21352.94
3 1938 20872.22
4 1950 47511.18
5 1954 29561.81
6 1958 23423.14

3. Metabolites

> mb <- read.csv("../data/metabolite.csv")</pre>

> head(mb)

	A alpha AAA c4 OH Pro Carnos	ine Creatinine DOPA Dopamine H	Histamine Kunurenine
1 Alzheimer 72.8 166 170 282 1.15	-	270 49.9 0.265 0.233	0.225 5.21
2 Alzheimer 93.4 138 142 217 1.05		350 48.8 0.252 NA	0.211 5.44
3 Alzheimer 68.6 161 158 208 1.00		998 30.4 0.268 NA	0.217 5.20
4 Alzheimer 94.1 129 162 201 1.10		675 80.1 0.264 0.234	0.209 5.80
5 Alzheimer 79.8 126 115 199 1.24		280 60.5 0.271 0.231	0.210 4.46
Met.SO Nitro.Tyr PEA Putrescine			
1 0.526 0.027 NA 0.068	-	-	5 1.13 18.2 0.059
2 0.387 NA NA 0.08			0 1.65 17.0 0.051
3 0.651 NA NA 0.260			9 1.57 12.6 0.083
4 0.389 NA NA 0.110			9 1.34 23.5 0.071
5 0.466 NA NA 0.118			9 1.24 13.6 0.139
C10.1 C10.2 C12 C12.DC C12.1	C14 C14.1 C14.1.OH C14.2		
1 0.312 0.038 0.030 0.042 0.290		0.006 0.046 0.008 0.009	0.007 0.005
2 0.288 0.039 0.038 0.038 0.265		0.009 0.070 0.009 0.013	0.006 0.006
3 0.357 0.054 0.032 0.048 0.302		0.009 0.076 0.011 0.019	0.010 0.005
4 0.317 0.040 0.045 0.048 0.275			0.008 0.006
5 0.472 0.074 0.056 0.079 0.394			0.014 0.012
C16.2.OH C18 C18.1 C18.1.OH (C5 C5.M.DC
	0.016 1.97 0.354 0.008 0.015		
	0.028 1.95 0.184 0.009 0.013		
	0.018 1.70 0.371 NA 0.012		
4 0.009 0.020 0.035 0.004 (0.033 2.10 0.278 0.010 0.017	0.110 0.077 0.031 0.14	45 0.034
5 0.025 0.031 0.034 0.012 0	0.017 5.62 0.436 0.029 0.035	0.106 0.099 0.069 0.14	41 0.094
C5.OHC3.DC.M. C5.1 C5.1.DC	C6C4.1.DC. C5.DCC6.OH.	C6.1 C7.DC C8 C9 lysoPC.a	a.C14.0
1 0.026 0.030 0.020	0.022 0.014 0	.018 0.011 0.062 0.016	2.23
2 0.026 0.024 0.021	0.030 0.018 0	.015 0.010 0.058 0.014	1.97
0 004 0 007 0 010	0.022 0.029 0		
3 0.024 0.037 0.018	0.022 0.029 0	.031 0.021 0.090 0.017	2.12
4 0.041 0.035 0.016		.031 0.021 0.090 0.017 .027 0.017 0.091 0.018	2.12 2.19
	0.029 0.016 0		
4 0.041 0.035 0.016	0.029 0.016 0 0.052 0.040 0	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041	2.19 1.88
4 0.041 0.035 0.016 5 0.058 0.073 0.049	0.029 0.016 0 0.052 0.040 0	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 D lysoPC.a.C18.1 lysoPC.a.C18.2	2.19 1.88 2 lysoPC.a.C20.3
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18.	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2	2.19 1.88 2 lysoPC.a.C20.3 7 1.830
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2 5 3.94 4.42	2.19 1.88 2 lysoPC.a.C20.3 7 1.830 2 0.958
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2° 5 3.94 4.42 1 7.73 8.00	2.19 1.88 2 lysoPC.a.C20.3 7 1.830 2 0.958 2 2.050
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53	0.029 0.016 0 0.052 0.040 0 lysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2° 5 3.94 4.42 1 7.73 8.02 1 7.22 7.62	2.19 1.88 2 lysoPC.a.C20.3 7 1.830 2 0.958 2 2.050 2 1.640
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39	0.029 0.016 0 0.052 0.040 0 lysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2° 5 3.94 4.42 1 7.73 8.02 1 7.22 7.62 6 5.39 3.60	2.19 1.88 2 lysoPC.a.C20.3 7 1.830 2 0.958 2 2.050 2 1.640 0 0.970
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 8.25 0.079	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2 5 3.94 4.42 1 7.73 8.02 1 7.22 7.62 6 5.39 3.66 1 lysoPC.a.C28.0 lysoPC.a.C28.3 3 0.108 0.041	2.19 1.88 2 lysoPC.a.C20.3 7 1.830 2 0.958 2 2.050 2 1.640 0 0.970 1 PC.aa.C24.0 2 0.082
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 8.25 0.079 2 4.60 0.059	0.029 0.016 0 0.052 0.040 0 lysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2 5 3.94 4.42 1 7.73 8.02 1 7.22 7.62 6 5.39 3.66 1 lysoPC.a.C28.0 lysoPC.a.C28.3 3 0.108 0.041	2.19 1.88 2 lysoPC.a.C20.3 7 1.830 2 0.958 2 2.050 2 1.640 0 0.970 1 PC.aa.C24.0 2 0.082
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 8.25 0.079	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2 5 3.94 4.4 1 7.73 8.0 1 7.22 7.6 6 5.39 3.6 1 lysoPC.a.C28.0 lysoPC.a.C28.3 0 0.108 0.075 2 0.076 0.058	2.19 1.88 2 lysoPC.a.C20.3 7 1.830 2 0.958 2 2.050 2 1.640 0 0.970 1 PC.aa.C24.0 2 0.082 8 0.065
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 8.25 0.079 2 4.60 0.059 3 9.84 0.075 4 6.75 0.066	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05 0.066 0.04 0.126 0.04	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 5 3.94 4.44 1 7.73 8.00 1 7.22 7.66 5 5.39 3.60 1 lysoPC.a.C28.0 lysoPC.a.C28.2 3 0.108 0.076 0 0.076 0.056 9 0.078 0.096 5 0.076 0.076	2.19 1.88 2 lysoPC.a.C20.3 7
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 8.25 0.079 2 4.60 0.059 3 9.84 0.075	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05 0.066 0.04 0.126 0.04	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 5 3.94 4.4 1 7.73 8.00 1 7.22 7.66 5 5.39 3.60 1 lysoPC.a.C28.0 lysoPC.a.C28.2 3 0.108 0.076 0 0.076 0.056 9 0.078 0.092 5 0.076 0.076	2.19 1.88 2 lysoPC.a.C20.3 7
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 8.25 0.079 2 4.60 0.059 3 9.84 0.075 4 6.75 0.066 5 6.26 0.084 PC.aa.C26.0 PC.aa.C28.1 PC.aa.C	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05 0.066 0.04 0.126 0.04 0.126 0.04 0.086 0.04 0.118 0.05	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2 5 3.94 4.4 1 7.73 8.0 1 7.22 7.6 5 5.39 3.6 1 lysoPC.a.C28.0 lysoPC.a.C28.3 3 0.108 0.07 2 0.076 0.05 9 0.078 0.092 0.076 0.076 0.076 0.076 0.076 0.076 0.076 0.076	2.19 1.88 2 lysoPC.a.C20.3 7
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 2 1 8.25 0.079 2 4.60 0.059 3 9.84 0.075 4 6.75 0.066 5 6.26 0.084 PC.aa.C26.0 PC.aa.C28.1 PC.aa.C21 1 0.438 0.571	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05 0.066 0.04 0.126 0.04 0.126 0.04 0.126 0.04 0.118 0.05 C30.0 PC.aa.C32.0 PC.aa.C32.	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 5 3.94 4.42 1 7.73 8.02 1 7.22 7.62 5 3.9 3.60 1 lysoPC.a.C28.0 lysoPC.a.C28.2 3 0.108 0.072 2 0.076 0.058 9 0.076 0.058 9 0.076 0.058 1 0.076 0.058 1 0.076 0.076 1 0.076 0.076 1 0.076 0.076 2 0.076 0.076 3 0.092 0.076	2.19 1.88 2 lysoPC.a.C20.3 7
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 1 8.25 0.079 2 4.60 0.059 3 9.84 0.075 4 6.75 0.066 5 6.26 0.084 PC.aa.C26.0 PC.aa.C28.1 PC.aa.C1 1 0.438 0.571 2 0.409 0.521	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05 0.066 0.04 0.126 0.04 0.126 0.04 0.126 0.04 0.118 0.05 0.086 0.04 0.118 0.05 0.086 0.04 0.118 0.05 0.006 0.04 0.118 0.05 0.007 0.018 0.04 0.118 0.05 0.008 0.04 0.118 0.05	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2 5 3.94 4.4 1 7.73 8.0 1 7.22 7.6 5.39 3.6 1 lysoPC.a.C28.0 lysoPC.a.C28.3 3 0.108 0.072 0 0.076 0.058 9 0.076 0.058 9 0.076 0.076 1 0.076 0.076 1 0.092 0.076 1 PC.aa.C32.2 PC.aa.C32.3 PC.aa 2 NA 0.092 0 NA 0.067	2.19 1.88 2 lysoPC.a.C20.3 7
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 8.25 0.079 2 4.60 0.059 3 9.84 0.075 4 6.75 0.066 5 6.26 0.084 PC.aa.C26.0 PC.aa.C28.1 PC.aa.C 1 0.438 0.571 2 0.409 0.521 3 0.458 0.605	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05 0.066 0.04 0.126 0.04 0.126 0.04 0.086 0.04 0.118 0.05 0.018 0.05 0.018 0.05 0.018 0.05 0.018 0.05 0.018 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04 0.196 0.04	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2 3.94 4.4 1 7.73 8.0 1 7.22 7.6 6 5.39 3.6 1 lysoPC.a.C28.0 lysoPC.a.C28.3 3 0.108 0.07 0 0.076 0.058 0 0.076 0.058 0 0.076 0.092 0 0.076 0.092 1 PC.aa.C32.2 PC.aa.C32.3 PC.aa 2 NA 0.092 NA 0.092 NA 0.067 NA 0.067	2.19 1.88 2 lysoPC.a.C20.3 7
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 8.25 0.079 2 4.60 0.059 3 9.84 0.075 4 6.75 0.066 5 6.26 0.084 PC.aa.C26.0 PC.aa.C28.1 PC.aa.C 1 0.438 0.571 2 0.409 0.521 3 0.458 0.605 4 0.486 0.685	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05 0.066 0.04 0.126 0.04 0.126 0.04 0.118 0.05 0.086 0.04 0.118 0.05 0.086 0.04 0.118 0.05 0.086 0.04 0.118 0.5 0.099 12.7 5.4 2.69 16.6 11.6 3.33 18.6 13.3	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2 5 3.94 4.4 1 7.73 8.00 1 7.22 7.60 6 5.39 3.66 1 lysoPC.a.C28.0 lysoPC.a.C28.3 3 0.108 0.07 2 0.076 0.053 9 0.078 0.092 0.076 0.076 0.092 0.076 1 PC.aa.C32.2 PC.aa.C32.3 PC.aa 0 NA 0.092 0 NA 0.067 NA 0.105	2.19 1.88 2 lysoPC.a.C20.3 7
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 8.25 0.079 2 4.60 0.059 3 9.84 0.075 4 6.75 0.066 5 6.26 0.084 PC.aa.C26.0 PC.aa.C28.1 PC.aa.C 1 0.438 0.571 2 0.409 0.521 3 0.458 0.605 4 0.486 0.685 5 0.401 0.513	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05 0.066 0.04 0.126 0.04 0.126 0.04 0.118 0.05 0.086 0.04 0.118 0.05 0.018 0.05 0.019 0.018 0.05 0.019 0.018 0.05	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2 5 3.94 4.4 1 7.73 8.00 1 7.22 7.62 5 5.39 3.60 1 lysoPC.a.C28.0 lysoPC.a.C28.3 3 0.108 0.07 2 0.076 0.058 9 0.078 0.092 0.076 0.076 0.092 0.076 0.092 0.076 0.092 0.076 0.092 0.076 0.092 0.076 0.092 0.076 0.092 0.076 0.092 0.076 0.092 0.076 0.092 0.076 0.092 0.076 0.092 0.076 0.092 0.076 0.093 0.092 0.076 0.094 0.095 0.095 0.095 0.096 0.076 0.097 0.097 0.098 0.099	2.19 1.88 2 lysoPC.a.C20.3 7
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 8.25 0.079 2 4.60 0.059 3 9.84 0.075 4 6.75 0.066 5 6.26 0.084 PC.aa.C26.0 PC.aa.C28.1 PC.aa.C 1 0.438 0.571 2 0.409 0.521 3 0.458 0.605 4 0.486 0.685 5 0.401 0.513 PC.aa.C34.3 PC.aa.C34.4 PC.aa.C	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05 0.066 0.04 0.126 0.04 0.126 0.04 0.126 0.04 0.118 0.05 0.05 0.05 0.05 0.05 0.05 0.05 0.05	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2 5 3.94 4.4 1 7.73 8.00 1 7.22 7.60 6 5.39 3.60 1 lysoPC.a.C28.0 lysoPC.a.C28.3 3 0.108 0.07 2 0.076 0.058 9 0.078 0.092 0.076 0.076 0.092 0.076 1 PC.aa.C32.2 PC.aa.C32.3 PC.aa 2 NA 0.092 0 NA 0.092 0 NA 0.067 0 NA 0.105 0 0.053 0.079 0 NA 0.105 0 0.053 0.079 0 NA 0.102 2 PC.aa.C36.3 PC.aa.C36.4 PC.aa	2.19 1.88 2 lysoPC.a.C20.3 7
4 0.041 0.035 0.016 5 0.058 0.073 0.049 lysoPC.a.C16.0 lysoPC.a.C16.1 1 37.9 2.66 2 22.1 1.31 3 33.7 2.53 4 32.8 2.39 5 24.5 1.27 lysoPC.a.C20.4 lysoPC.a.C24.0 1 8.25 0.079 2 4.60 0.059 3 9.84 0.075 4 6.75 0.066 5 6.26 0.084 PC.aa.C26.0 PC.aa.C28.1 PC.aa.C 1 0.438 0.571 2 0.409 0.521 3 0.458 0.605 4 0.486 0.685 5 0.401 0.513	0.029 0.016 0 0.052 0.040 0 LysoPC.a.C17.0 lysoPC.a.C18. 0.446 9.0 0.270 5.3 0.399 7.5 0.323 7.2 0.382 6.6 LysoPC.a.C26.0 lysoPC.a.C26. 0.113 0.05 0.066 0.04 0.126 0.04 0.126 0.04 0.118 0.05 0.086 0.04 0.118 0.05 0.018 0.05 0.019 0.018 0.05 0.019 0.018 0.05	.027 0.017 0.091 0.018 .040 0.036 0.192 0.041 0 lysoPC.a.C18.1 lysoPC.a.C18.2 0 8.58 7.2 5 3.94 4.4 1 7.73 8.0 1 7.22 7.6 6 5.39 3.6 1 lysoPC.a.C28.0 lysoPC.a.C28.3 3 0.108 0.07 2 0.076 0.05 9 0.076 0.05 9 0.076 0.07 3 0.092 0.07 1 PC.aa.C32.2 PC.aa.C32.3 PC.aa 2 NA 0.092 0 NA 0.092 0 NA 0.105 0 0.053 0.079 0 NA 0.105 0 0.053 0.079 0 NA 0.102 2 PC.aa.C36.3 PC.aa.C36.4 PC.aa 4 42.7 120.0	2.19 1.88 2 lysoPC.a.C20.3 7

3	1.930	0.210	2.30	19.9	44.	43.9	146.0	2.09	0.057
4	1.590	0.190	2.57	20.9	48.	3 41.2	122.0	1.76	0.070
5	0.709	0.135	1.83	20.5	28.	5 21.9	98.1	1.70	0.048
						5 PC.aa.C40.1			
1		32.1	95.1						3.48
1	1.230				41.			0.491	
2	0.946	21.9	78.9		25.			0.358	3.39
3	1.210	34.5	107.0	17.50	36.	0.212	0.118	0.395	3.56
4	1.160	28.7	92.7	14.30	29.	0.220	0.097	0.433	3.59
5	1.100	23.3	101.0	13.80	36.	0.165	0.044	0.525	3.37
-						PC.aa.C42.4			
-					0.10				0.173
1	5.66	21.8	0.364					0.291	
2	4.08	14.2	0.419	0.216	0.10	0.336	0.317	0.248	0.147
3	5.34	16.7	0.476	0.281	0.11	0.300	0.206	0.267	0.209
4	5.06	14.0	0.427	0.223	0.11	0.268	0.267	0.254	0.223
5	5.29	22.5	0.125		0.08			0.280	0.095
J						PC.ae.C34.1			
1	0.027	0.022	1.65		0.88			0.813	0.498
2	0.024	0.020	2.01	0.360	0.76	3 2.68	2.32	0.905	0.398
3	0.046	0.030	2.40	0.477	0.93	3 4.04	2.95	1.030	0.554
4	0.049	0.023	2.47		0.96			1.020	0.552
5	0.082	0.023	1.72		1.06			0.722	0.553
	PC.ae.C36.1	PC.ae.C36.2	PC.ae.C36.3	PC.ae.C36.4	PC.ae.C36.	PC.ae.C38.0	PC.ae.C38.1	PC.ae.C38.2	PC.ae.C38.3
1	5.64	1.90	1.170	6.96	4.7	0.474	0.287	0.538	2.66
2	3.89	1.54	0.873	6.40	5.3	0.325	NA	0.127	1.80
3	5.95	2.29			6.6			0.154	2.87
4	4.75	2.01	1.350		5.9			0.144	1.97
5	5.95	1.47	0.760		4.0			0.246	1.80
	PC.ae.C38.4	PC.ae.C38.5	PC.ae.C38.6	PC.ae.C40.1	PC.ae.C40.	PC.ae.C40.3	PC.ae.C40.4	PC.ae.C40.5	PC.ae.C40.6
1	6.33	5.51	1.95	0.574	0.57	0.940	1.76	1.77	1.59
2	5.37	4.49	1.63	0.281	0.49	0.702	1.43	1.55	1.20
3	7.06	5.64	1.98		0.65			1.64	1.49
4	5.99	5.63	1.97		0.54			1.62	1.25
5	5.45	4.34	1.51		0.43			1.25	1.47
	PC.ae.C42.0	PC.ae.C42.1	PC.ae.C42.2	PC.ae.C42.3	PC.ae.C42.	PC.ae.C42.5	PC.ae.C44.3	PC.ae.C44.4	PC.ae.C44.5
1	0.629	0.316	0.192	0.277	0.26	0.888	0.065	0.168	0.536
2	0.616	0.260	0.157	0.200	0.31	L 0.840	0.071	0.220	0.470
3	0.686	0.356	0.241		0.31			0.228	0.565
4	0.637	0.299			0.39			0.237	0.517
5	0.660	0.355	0.138	0.174	0.16	0.513	0.081	0.154	0.178
	PC.ae.C44.6	SMOHC14	.1 SMOHC	16.1 SMOH.	.C22.1 SM	DHC22.2 SM.	.OHC24.1 SM	4.C16.0 SM.C	16.1 SM.C18.0
1	0.494	1.4	20	1.33	2.07	1.86	0.597	44.9	7.99 14.5
2	0.515	1.3	90	1.25	2.47	2.20	0.640	42.1	6.88 12.7
3	0.603	1.8		1.58	2.69	2.63	0.665		8.91 14.6
4	0.611	1.7		1.48	2.97	2.84	0.682		8.61 17.2
5	0.134	0.9	87	1.48	1.96	1.74	0.478	40.6	5.86 13.0
	SM.C18.1 SM.	C20.2 SM.C2	4.0 SM.C24.1	SM.C26.0 SM	.C26.1 H1 1	H1 Urea N	L.Arginine N	L.Leucine N	EDTAca N
1	10.40	0.290 12	.20 27.3	0.147	0.337 3356	3356 NA	NA	NA	NA
2	8.52		.40 25.6			2509 201.9	22.5	35.3	2.0
2							21.0		
3		0.304 11		0.163		2661 193.3		25.4	1.8
4		0.261 11				2652 500.8		27.1	2.5
5	8.34	0.196 9	.29 20.5	0.111	0.283 2258	2258 132.5	13.2	57.9	2.5
	X2.Hydroxybu	tvrate X3.H	vdroxvbutvra	te Acetate A	cetoacetate	Acetone Beta	ine Carnitine	e Choline Cre	eatine
1	1 1	NA		NA NA	NA	NA	NA NA		NA
2		12.40		.5 13.2	5.7		2.0 8.7		14.5
3		11.33	11		9.3		9.1 15.3		17.8
4		12.70	7	.2 9.8	4.8	4.0 1	3.9 7.7	7 11.8	14.7
5		35.20	44	.7 20.2	18.9	18.9 3	3.9 18.5	5 27.7	35.4
	Dimethvl.sul					nine Isobutyr			
1		NA NA		NA 1		_		NA NA	NA
2		4.7 16.						1.9 1171.6	10.4
3		2.1 8.3						2.5 1938.1	13.1
4		1.3 6.	4 14.4	629.5 322	. 0	8.6	2.5	4.4 1037.7	7.6
5		5.5 13.0	0 40.0 1	618.0 271	. 6	0.0	6.1 11	1.2 2199.9	11.7
	[reached 'ma	x' / getOnt	ion("max.pri			I			
		. 3	,	,		•			

a. Alzheimer's patients

b. Missing values per column

```
> head(colSums(is.na(mb)))
Label Phe Pro Ser Thr ADMA
     0     0     0     0     0
```

c. New data frame with rows missing **Dopamine** value

>	head(mb1 <- mb[!is	s.na(mb\$Dopamin	e),])					
	Label Phe Pro	o Ser Thr ADMA	alpha.AAA c4.OH	.Pro Carnosi	ne Creatinine	DOPA Dopami	ine Histamin	e Kynurenine
1	Alzheimer 72.8 166	6 170 282 1.15	0.760 0	1.2	70 49.9	0.265 0.2	233 0.22	5 5.21
4	Alzheimer 94.1 129	9 162 201 1.10	0.795	NA 0.6	75 80.1	0.264 0.2	234 0.20	9 5.80
5	Alzheimer 79.8 126	6 115 199 1.24	1.360	NA 1.2	80 60.5	0.271 0.2	231 0.21	0 4.46
8	Healthy 83.6 119	9 135 268 1.18	0.779 0	0.6	47 30.6	0.275 0.2	244 0.21	4 5.66
9	Healthy 73.7 124	4 145 307 1.17	0.785 0	0.186	90 39.8	0.259 0.2	233 0.21	0 6.36
	Met.SO Nitro.Tyr B	PEA Putrescine	Sarcosine Serot			4.OH.Pro Ta	urine SDMA	C0 C10
1	0.526 0.027	NA 0.068	17.8 0	0.147 0.1	188 NA	24.0	125 1.13 1	8.2 0.059
4	0.389 NA	NA 0.110	18.7 0	0.255 0.	353 NA	23.1	159 1.34 2	3.5 0.071
5	0.466 NA	NA 0.118		0.390 0.	473 NA	26.9	149 1.24 1	3.6 0.139
8	0.245 0.002	NA 0.161	23.3 0	0.215 0.3	276 NA	10.7	133 1.04 1	3.3 0.051
9	0.413 NA				327 NA	16.0	215 1.24 1	
		C12.DC C12.1	C14 C14.1 C14.			C16.OH C16.		
	0.312 0.038 0.030			.008 0.008	0.006 0.046			
	0.317 0.040 0.045			0.010 0.013	0.011 0.074			
	0.472 0.074 0.056			0.016 0.025	0.017 0.062	NA 0.024		
	0.217 0.030 0.041			0.007 0.006	0.007 0.060			
9	0.258 0.036 0.037			0.007 0.007	0.007 0.054			
		8.1 C18.1.OH C1		C3.OH C3.1		C4.OH. C4.1	C5 C5.M.	
1	0.013 0.013 0.0		016 1.97 0.354			0.045 0.025		
4	0.009 0.020 0.0		033 2.10 0.278			0.077 0.031		
5	0.025 0.031 0.0					0.099 0.069		
8	0.008 0.020 0.0		019 1.66 0.258			0.047 0.021		
9	0.009 0.014 0.0		016 2.21 0.233			0.029 0.024		24
1	C5.OHC3.DC.M. (-	PC.a.C14.0	
1	0.026 0.		0.022 0.029		018 0.011 0.06		2.23	
5	0.041 0. 0.058 0.		0.029		027 0.017 0.09 040 0.036 0.19		1.88	
8	0.023 0.		0.032	0.040 0.0	NA 0.009 0.03		2.13	
9	0.023 0.		0.036		015 0.013 0.06		2.13	
9	lysoPC.a.C16.0 lys							
1	37.9	2.66	0.446	9.00	-	-	7.27	1.83
4	32.8	2.39	0.323	7.21			7.62	1.64
5	24.5	1.27	0.382	6.66			3.60	0.97
8	33.7	3.09	0.455	6.96			7.53	2.35
9	36.0	3.46	0.435	7.27			6.75	2.08
	lysoPC.a.C20.4 lys							
1	8.25	0.079	0.113	0.053	_	_		0.082
4	6.75	0.066	0.086	0.045		76 (0.076	0.076
5	6.26	0.084	0.118	0.053				0.069
8	8.73	0.061	0.083	0.047				0.082
9	7.82	0.068	0.083	0.037	0.09	96 (0.061	0.064
	PC.aa.C26.0 PC.aa.	.C28.1 PC.aa.C3	0.0 PC.aa.C32.0	PC.aa.C32.1	PC.aa.C32.2 E	C.aa.C32.3 1	PC.aa.C34.1	PC.aa.C34.2
1	0.438	0.571 2	.35 11.4	9.22	NA	0.092	109.0	71.0
4	0.486	0.685 3	.33 18.6	13.30	0.053	0.079	106.0	93.6
5	0.401	0.513 1	.78 13.8	5.03	NA	0.102	83.4	35.9
8	0.424	0.605 2	.32 12.1	11.50	NA	0.093	83.6	60.6
9	0.430	0.486 2	.05 10.4	11.40	NA	0.082	89.6	55.1
	PC.aa.C34.3 PC.aa.	.C34.4 PC.aa.C3	6.0 PC.aa.C36.1	PC.aa.C36.2	PC.aa.C36.3 H	C.aa.C36.4 1	PC.aa.C36.5	PC.aa.C36.6
1	1.430	0.200 2	.38 21.7	42.4	42.7	120.0	1.86	0.084
4	1.590	0.190 2	.57 20.9	48.8	41.2	122.0	1.76	0.070
5	0.709	0.135 1	.83 20.5	28.5	21.9	98.1	1.70	0.048
8	1.580	0.251 2	.16 18.4	34.4	41.5	110.0	2.03	0.106
9	1.390		.62 18.3			102.0	1.77	0.081
	PC.aa.C38.0 PC.aa.	.C38.3 PC.aa.C3	8.4 PC.aa.C38.5	PC.aa.C38.6	PC.aa.C40.1 E		PC.aa.C40.3	PC.aa.C40.4
1	1.230		5.1 16.8	41.6		0.074	0.491	3.48
4	1.160		2.7 14.3			0.097	0.433	3.59
5	1.100	23.3 10	1.0 13.8	36.2	0.165	0.044	0.525	3.37

8	1.150	31.3	81.7	14.5	42.8	0.225	0.099	0.384	4.02
9	0.902	31.1	75.9	13.6	37.6			0.298	2.88
						PC.aa.C42.4			
1	5.66	21.8	0.364	0.226	0.108			0.291	0.173
4	5.06	14.0	0.427	0.223	0.100			0.254	0.223
5	5.29	22.5	0.125	0.223	0.083		0.205	0.280	0.223
8									
	5.49	20.6	0.365	0.193	0.089		0.237	0.288	0.212
9	4.88	17.5	0.396	0.216	0.086		0.206	0.223	0.179
						PC.ae.C34.1			
1	0.027	0.022	1.65	0.371	0.880		2.48	0.813	0.498
4	0.049	0.023		0.459	0.964			1.020	0.552
5	0.082	0.023	1.72	0.316	1.060		1.70	0.722	0.553
8	0.028	0.033		0.335	1.140		2.28	0.868	0.479
9	0.012	0.022	1.53	0.291	0.683		2.03	0.663	0.384
	PC.ae.C36.1					PC.ae.C38.0			
1	5.64	1.90	1.17	6.96	4.79		0.287	0.538	2.66
4	4.75	2.01	1.35	8.36	5.97	0.397	0.022	0.144	1.97
5	5.95	1.47	0.76	4.78	4.00	0.430	0.271	0.246	1.80
8	5.65	1.97	1.25	7.15	4.04	0.550	0.078	0.559	2.90
9	4.79	1.54	1.12	6.43	3.32	0.442	NA	0.224	2.53
	PC.ae.C38.4	PC.ae.C38.5	PC.ae.C38.6	PC.ae.C40.1	PC.ae.C40.2	PC.ae.C40.3	PC.ae.C40.4	PC.ae.C40.5	PC.ae.C40.6
1	6.33	5.51	1.95	0.574	0.575	0.940	1.76	1.77	1.59
4	5.99	5.63	1.97	0.425	0.540	0.742	1.45	1.62	1.25
5	5.45	4.34	1.51	0.430	0.432			1.25	1.47
8	5.73	4.53		0.584	0.499		1.84	1.53	1.46
9	5.03	3.82	1.28	0.472	0.555			1.34	1.21
						PC.ae.C42.5			
1	0.629	0.316	0.192	0.277			0.065	0.168	0.536
4	0.637	0.299		0.208	0.392			0.237	0.517
5	0.660	0.355	0.138	0.174	0.162		0.081	0.154	0.178
8	0.631	0.271	0.186	0.282	0.333		0.085	0.183	0.534
9	0.645	0.264	0.168	0.229	0.319		0.069	0.184	0.671
									16.1 SM.C18.0
1	0.494	1.4		.330	2.07	1.86	0.597		7.99 14.5
4	0.611	1.7		.480	2.97	2.84	0.682		3.61 17.2
5	0.134	0.9		.480	1.96	1.74	0.478		5.86 13.0
8	0.429	1.5		.160	2.98	2.59	0.631		7.92 11.9
9	0.460	1.2		.984	2.21	2.07	0.507		6.65 12.0
			4.0 SM.C24.1		_	_	L.Arginine_N	_	_
1	10.40		.20 27.3	0.147	0.337 3356		NA 1600	NA	NA
4	11.50		.80 27.9	0.138	0.353 2652		16.0	27.1	2.5
5	8.34		.29 20.5	0.111	0.283 2258		13.2	57.9	2.5
8	9.59		.36 18.8	0.117	0.227 2464		49.8	63.9	0.0
9	8.48		.30 23.6	0.090		2725 255.8	39.0	64.6	2.7
	X2.Hydroxybu					Acetone Beta			
1		NA		NA NA	NA	NA	NA NA		NA
4		12.7	7.		4.8		3.9 7.7		14.7
5		35.2	44.		18.9		3.9 18.5		35.4
8		21.7	20.	.9 19.5	15.4	6.6 3	5.3 13.0	21.5	25.9
9		17.1	37.	.9 20.0	22.0	9.3 1	2.0 14.4	15.4	25.3
	Dimethyl.sul	fone Ethano	l Formate Glu	cose Glycer	ol Hypoxanth	ine Isobutyr	ate Isopropar	nol Lactate M	Malonate
1		NA N	A NA	NA 1	NA	NA	NA	NA NA	NA
4		1.3 6.	4 14.4 6	529.5 322	. 0	8.6	2.5	1.4 1037.7	7.6
5		5.5 13.0						1.2 2199.9	11.7
8		5.4 10.2						1.4 1661.4	11.0
9		3.5 5.1						5.7 2048.5	8.0
	[reached 'ma		ion("max.prir						
		. 5		,					

d. Median c4-OH-Pro value if missing

- > mb2 <- median(mb1\$c4.OH.Pro, na.rm = TRUE)
- > mb1\$c4.OH.Pro[is.na(mb1\$c4.OH.Pro)] <- mb2 > head(mb1)

-	nead (not)														
	Label	Phe	Pro	Ser	Thr	ADMA	alpha.AAA	c4.OH.Pro	Carnosine	Creatinine	DOPA	Dopamine	${\tt Histamine}$	Kynurenine	
	l Alzheimer	72.8	166	170	282	1.15	0.760	0.236	1.270	49.9	0.265	0.233	0.225	5.21	
4	Alzheimer	94.1	129	162	201	1.10	0.795	0.199	0.675	80.1	0.264	0.234	0.209	5.80	
ļ	5 Alzheimer	79.8	126	115	199	1.24	1.360	0.199	1.280	60.5	0.271	0.231	0.210	4.46	
8	B Healthy	83.6	119	135	268	1.18	0.779	0.215	0.647	30.6	0.275	0.244	0.214	5.66	
	Healthy	73.7	124	145	307	1.17	0.785	0.186	0.590	39.8	0.259	0.233	0.210	6.36	

```
Met.SO Nitro.Tyr PEA Putrescine Sarcosine Serotonin Spermidine Spermine t4.OH.Pro Taurine SDMA C0 C10
        0.027 NA 0.068 17.8 0.147 0.188 NA 24.0 125 1.13 18.2 0.059
           NA NA
                               18.7
                                      0.255
                                                0.353
                                                                23.1
                                                                       159 1 34 23 5 0 071
4
 0.389
                      0.110
                                                          NA
5 0.466
            NA NA
                    0.118
                            22.5
                                    0.390 0.473
                                                          NA
                                                                26.9
                                                                      149 1.24 13.6 0.139
                                    0.215
                                                                      133 1.04 13.3 0.051
                                             0.276
0.327
          0.002 NA
                      0.161
                               23.3
                                                         NA
                                                                10.7
8 0.245
                               22.1
                                      0.166
                                                          NA
                                                                16.0
                                                                        215 1.24 15.8 0.061
 0.413
            NA NA
                      0.121
 C10.1 C10.2 C12 C12.DC C12.1 C14 C14.1 C14.1.OH C14.2 C14.2.OH C16 C16.OH C16.1 C16.1.OH C16.2
1 0.312 0.038 0.030 0.042 0.290 0.023 0.019 0.008 0.008 0.006 0.046 0.008 0.009 0.007 0.005
4 0.317 0.040 0.045 0.048 0.275 0.026 0.028 0.010 0.013 5 0.472 0.074 0.056 0.079 0.394 0.034 0.043 0.016 0.025
                                                   0.011 0.074 0.011 0.015
                                                                          0.008.0.006
                                                 0.017 0.062 NA 0.024
                                                                         0.014 0.012
8 0.217 0.030 0.041 0.035 0.174 0.024 0.017 0.007 0.006
                                                  0.007 0.060 0.006 0.010
                                                                         0.005 0.004
9 0.258 0.036 0.037 0.038 0.228 0.022 0.018 0.007 0.007
                                                  0.007 0.054 0.005 0.012
                                                                         0.005 0.005
 C16.2.OH C18 C18.1 C18.1.OH C18.2 C2 C3 C3.OH C3.1
                                                   C4 C3.DC..C4.OH. C4.1
                                                                         C5 C5.M.DC
                                                          0.045 0.025 0.094 0.023
   0.004 0.033 2.10 0.278 0.010 0.017 0.110
                                                             0.077 0.031 0.145 0.034
  0.009 0.020 0.035
                   0.012 0.017 5.62 0.436 0.029 0.035 0.106
   0.025 0.031 0.034
                                                            0.099 0.069 0.141 0.094
   0.008 0.020 0.025
                     0.004 0.019 1.66 0.258 0.008 0.012 0.082
                                                             0.047 0.021 0.107
                                                                             0.023
                                                            0.029 0.024 0.127 0.024
                    0.003 0.016 2.21 0.233 0.008 0.014 0.088
  0.009 0.014 0.026
 C5.OH..C3.DC.M. C5.1 C5.1.DC C6..C4.1.DC. C5.DC..C6.OH. C6.1 C7.DC C8 C9 lysoPC.a.C14.0
         0.026 0.030 0.020 0.022
0.041 0.035 0.016 0.029
                                        0.014 0.018 0.011 0.062 0.016
                                          0.016 0.027 0.017 0.091 0.018
                                                                            2 19
         0.058 0.073 0.049
                              0.052
                                          0.040 0.040 0.036 0.192 0.041
                            0.036
                                         0.011 NA 0.009 0.062 0.011
         0.023 0.021 0.017
                                                                           2.13
         0.024 0.025 0.016
                               0.026
                                          0.018 0.015 0.013 0.064 0.014
                                                                            2.10
 lysoPC.a.C16.0 lysoPC.a.C16.1 lysoPC.a.C17.0 lysoPC.a.C18.0 lysoPC.a.C18.1 lysoPC.a.C18.2 lysoPC.a.C20.3
    37.9
              2.66 0.446 9.00 8.58 7.27 1.83
         32.8
                     2 39
                                 0.323
                                              7 21
                                                          7 22
                                                                       7 62
         24.5
                     1.27
                                0.382
                                              6.66
                                                          5.39
                                                                       3.60
                                                                                   0.97
                               0.455
         33.7
                     3.09
                                                          7.31
                                                                      7.53
                                                                                   2.35
                                             6.96
         36.0
                     3.46
                               0.435
                                             7.27
                                                         8.11
                                                                      6.75
 lysoPC.a.C20.4 lysoPC.a.C24.0 lysoPC.a.C26.0 lysoPC.a.C26.1 lysoPC.a.C28.0 lysoPC.a.C28.1 PC.aa.C24.0
    8.25 0.079 0.113 0.053 0.108 0.072 0.082
6.75 0.066 0.086 0.045 0.076 0.076 0.076
                                            0.053 0.092
                                0.118
                                                                     0.072
                    0.084
         6 26
                                                                               0.069
         8.73
                    0.061
                                 0.083
                                             0.047
                                                         0.124
                                                                      0.078
                                                                                0.082
                                            0.037 0.096
                0.068
                               0.083
                                                                     0.061
         7.82
                                                                                0.064
 PC.aa.C26.0 PC.aa.C28.1 PC.aa.C30.0 PC.aa.C32.0 PC.aa.C32.1 PC.aa.C32.2 PC.aa.C32.3 PC.aa.C34.1 PC.aa.C34.2
    0.438 0.571 2.35 11.4 9.22 NA 0.092 109.0
1
      0.486
               0.685
                          3.33
                                    18.6
                                             13.30
                                                       0.053
                                                                 0.079
                                                                           106.0
4
                                                                                      93.6
                                             5.03
                                                       NA
                                                                0.102
     0.401
              0.513
                         1.78
                                   13.8
                                                                           83.4
                                                                                      35.9
5
                                                                         83.6
              0.605
                      2.32
2.05
                                 12.1
10.4
                                         11.50 NA
11.40 NA
                                                         NA 0.093
NA 0.082
     0.424
                                                                                      60.6
      0.430
               0.486
                                                                           89.6
                                                                                      55.1
 PC.aa.C34.3 PC.aa.C34.4 PC.aa.C36.0 PC.aa.C36.1 PC.aa.C36.2 PC.aa.C36.3 PC.aa.C36.4 PC.aa.C36.5 PC.aa.C36.6
     1.430
           0.200 2.38 21.7 42.4 42.7 120.0 1.86 0.084
                                                                122.0
      1 590
               0.190
                          2.57
                                    20.9
                                              48.8
                                                        41 2
                                                                           1 76
                                                                                     0.070
      0.709
                0.135
                          1.83
                                    20.5
                                              28.5
                                                        21.9
                                                                  98.1
                                                                            1.70
                                 18.4 34.4 41.5 110.0
18.3 32.0 41.8 102.0
              0.251
     1.580
                          2 16
                                                                           2 03
                                                                                    0.106
8
     1.390
               0.221
                         1.62
                                                                           1.77
                                                                                     0.081
 PC.aa.C38.0 PC.aa.C38.3 PC.aa.C38.4 PC.aa.C38.5 PC.aa.C38.6 PC.aa.C40.1 PC.aa.C40.2 PC.aa.C40.3 PC.aa.C40.4
                      95.1
                               16.8 41.6 0.195 0.074 0.491
14.3 29.9 0.220 0.097 0.433
     1.230
                32.1
      1.160
                28.7
                          92.7
                                                      0.165 0.044
0.225 0.099
0.181
                                                                                      3.59
                                         36.2
42.8
                                                   0.165
                                                                         0.525
     1.100
                23.3
                        101.0
                                   13.8
                                                                                     3.37
5
      1.150
                 31.3
                          81.7
                                    14.5
                                                                          0.384
8
                                                                                      4 02
9
      0.902
                31.1
                          75.9
                                    13.6
                                                                           0.298
                                                                                      2.88
 PC.aa.C40.5 PC.aa.C40.6 PC.aa.C42.0 PC.aa.C42.1 PC.aa.C42.2 PC.aa.C42.4 PC.aa.C42.5 PC.aa.C42.6 PC.ae.C30.0
                                                                                 0.173
      5.66
            21.8 0.364 0.226 0.108 0.272 0.272 0.291
       5.06
                 14.0
                         0.427
                                   0.223
                                             0.119
                                                       0.268
                                                                 0.267
                                                                           0.254
                        0.125
                                            0.083
                                                      0.206
                                                                0.205
                22 5
                                  0.095
                                                                          0.280
                                                                                    0.095
5
      5 29
                        0.365
                                  0.193
                                            0.089
                                                      0.266
                                                                0.237
      5.49
                20.6
                                                                          0.288
                                                                                    0.212
      4.88
                17.5
                         0.396
                                   0.216
                                            0.086
                                                      0.215
                                                                0.206
                                                                          0.223
                                                                                     0.179
 PC.ae.C30.1 PC.ae.C30.2 PC.ae.C32.1 PC.ae.C32.2 PC.ae.C34.0 PC.ae.C34.1 PC.ae.C34.2 PC.ae.C34.3 PC.ae.C36.0
     0.027
             0.022 1.65 0.371 0.880 3.66 2.48 0.813 0.498
      0.049
                0.023
                          2.47
                                   0.459
                                             0.964
                                                        4.06
                                                                  3.09
                                                                          1.020
                                                                                     0.552
                                  0.316
                                                                1.70
                                            1.060
1.140
      0.082
               0.023
                          1.72
                                                        3.28
                                                                           0.722
                                                                                     0.553
Ω
      0.028
               0.033
                          1.68
                                   0.335
                                                        3.51
                                                                  2.28
                                                                           0.868
                                                                                    0 479
                                 0.291
                                                      3.20
                                                                2.03
                         1.53
                                            0.683
     0.012
               0.022
                                                                          0.663
 PC.ae.C36.1 PC.ae.C36.2 PC.ae.C36.3 PC.ae.C36.4 PC.ae.C36.5 PC.ae.C38.0 PC.ae.C38.1 PC.ae.C38.2 PC.ae.C38.3
    5.64 1.90 1.17 6.96 4.79 0.474 0.287 0.538 2.66
                                              5.97
                                                       0.397
4
       4.75
                 2.01
                          1.35
                                    8.36
                                                                 0.022
                                                                           0.144
                                                                                      1.97
                        0.76
                                  4.78
                                          4.00
                                                   0.430 0.271
                                                                          0.246
      5.95
               1.47
                                   7.15
                                                               0.078
      5 65
               1 97
                         1.25
                                            4.04
                                                      0.550
                                                                          0.559
                                                                                     2.90
```

9	4.79	1.	54	1.1	.2	6.43		3.32		0.442	NA	L	0.224		2.53
	PC.ae.C38.4	PC.ae.C38	.5 PC	.ae.C38	6 PC.	ae.C40.1	PC.ae	.C40.2	PC.a	e.C40.3	PC.ae.C40.4	PC.ae	.C40.5	PC.ae	.C40.6
1	6.33	5.	51	1.9	5	0.574		0.575		0.940	1.76	i	1.77		1.59
4	5.99	5.	63	1.9	7	0.425		0.540		0.742	1.45	i	1.62		1.25
5	5.45	4.	34	1.5	1	0.430		0.432		0.632	1.10	1	1.25		1.47
8	5.73	4.	53	1.7	1	0.584		0.499		0.991	1.84		1.53		1.46
9	5.03	3.	82	1.2	:8	0.472		0.555		0.737	1.35		1.34		1.21
	PC.ae.C42.0	PC.ae.C42	.1 PC	.ae.C42	2 PC.	ae.C42.3	PC.ae	.C42.4	PC.a	e.C42.5	PC.ae.C44.3	PC.ae	.C44.4	PC.ae	.C44.5
1	0.629	0.3	16	0.19	2	0.277		0.264		0.888	0.065		0.168		0.536
4	0.637	0.2	99	0.15	9	0.208		0.392		0.863	0.069	1	0.237		0.517
5	0.660	0.3	55	0.13	8	0.174		0.162		0.513	0.081		0.154		0.178
8	0.631	0.2	71	0.18	16	0.282		0.333		0.861	0.085	i	0.183		0.534
9	0.645	0.2	64	0.16	8	0.229		0.319		0.925	0.069	1	0.184		0.671
	PC.ae.C44.6	SMOH	14.1	SMOH.	C16.1	SMOH.	.C22.1	SMC	HC2	22.2 SM.	.OHC24.1 S	M.C16.	0 SM.C	16.1 SI	M.C18.0
1	0.494	-	.420		1.330		2.07		1	.86	0.597	44.	9	7.99	14.5
4	0.611	-	.720		1.480		2.97		2	2.84	0.682	52.	4	8.61	17.2
5	0.134	(.987		1.480		1.96		1	.74	0.478	40.	6	5.86	13.0
8	0.429		.500		1.160		2.98		2	2.59	0.631	37.	9	7.92	11.9
9	0.460	-	.230		0.984		2.21		2	2.07	0.507	37.	3	6.65	12.0
	SM.C18.1 SM.	.C20.2 SM	C24.0	SM.C24	1 SM.	C26.0 SM	.C26.1	H1 1	Н1	Urea N	L.Arginine N	L.Leu	cine N	EDTAc	a N
1	10.40	0.290	12.20	27.	3 (0.147	0.337	3356	3356	NA	NA		NA		NA
4	11.50	0.261	11.80	27.	9 (0.138	0.353	2652	2652	500.8	16.0		27.1	:	2.5
5	8.34	0.196	9.29	20.	5 (0.111	0.283	2258	2258	132.5	13.2		57.9	:	2.5
8	9.59	0.199	9.36	18.	8 (0.117	0.227	2464	2464	182.3	49.8		63.9		0.0
9	8.48	0.183	10.30	23.	6	0.090	0.268	2725	2725	255.8	39.0		64.6	:	2.7
	X2.Hydroxybu	ityrate X3	.Hydr	oxybuty	ate A	cetate A	cetoac	etate	Aceto	ne Beta	ine Carnitin	e Chol	ine Cr	eatine	
1		NA			NA	NA		NA		NA	NA N	ΙA	NA	NA	
4		12.7			7.2	9.8		4.8	4	1.0 1	3.9 7.	7 1	1.8	14.7	
5		35.2		4	4.7	20.2		18.9	18	3.9	3.9 18.	5 2	7.7	35.4	
8		21.7		2	0.9	19.5		15.4	6	5.6 3	5.3 13.	0 2	1.5	25.9	
9		17.1		3	7.9	20.0		22.0	9	3.3 1	2.0 14.	4 1	5.4	25.3	
	Dimethyl.sul	fone Etha	nol F	ormate (lucos	e Glycer	ol Hypo	oxanth	ine 1	sobutyr	ate Isopropa	nol La	ctate	Malona	te
1		NA	NA	NA	N	A	NA		NA		NA	NA	NA	1	NA
4		1.3	6.4	14.4	629.	322	.0		8.6		2.5	4.4 1	037.7	7	. 6
5		5.5	3.0	40.0	1618.	271	. 6		0.0		6.1 1	1.2 2	199.9	11	.7
8		5.4	0.2	23.2	2120.	5 406	.5		5.8		4.5	4.4 1	661.4	11	.0
9		3.5	5.1	25.0	1644.	2 479	. 9		5.6		5.9	6.7 2	048.5	8	.0
	[reached 'max' / getOption("max.print") omitted 1 rows]														

e. Drop columns with > 25% missing values

0.016 0.027 0.017 0.091 0.018

> mb3 <- colSums(is.na(mb1)) <= 0.25 * nrow(mb1)

0.029

```
> head(mb1 <- mb1[, mb3])
    Label Phe Pro Ser Thr ADMA alpha.AAA c4.OH.Pro Carnosine Creatinine DOPA Dopamine Histamine Kynurenine
                                                         49.9 0.265
1 Alzheimer 72.8 166 170 282 1.15 0.760 0.236 1.270
                                                                         0.233 0.225 5.21
                                 0.795
4 Alzheimer 94.1 129 162 201 1.10
                                          0.199
                                                   0.675
                                                              80.1 0.264
                                                                          0.234
```

5 Alzheimer 79.8 126 115 199 1.24 1.360 1.280 60.5 0.271 0.199 0.231 0.210 4.46 8 Healthy 83.6 119 135 268 1.18 0.779 0.215 0.647 30.6 0.275 0.244 0.214 0.210 9 Healthy 73.7 124 145 307 1.17 0.785 0.590 39.8 0.259 0.233 0.186 6.36 Met.SO Putrescine Sarcosine Serotonin Spermidine t4.0H.Pro Taurine SDMA C0 C10 C10.1 C10.2 C12 C12.DC 17.8 0.147 0.188 24.0 125 1.13 18.2 0.059 0.312 0.038 0.030 0.042 1 0.526 0.068 4 0.389 0.110 18.7 0.255 0.353 23.1 159 1.34 23.5 0.071 0.317 0.040 0.045 0.048 0.390 26.9 149 1.24 13.6 0.139 0.472 0.074 0.056 0.079 5 0.466 0.118 22.5 0.473 8 0.245 0.161 23.3 0.215 0.276 10.7 133 1.04 13.3 0.051 0.217 0.030 0.041 0.035 9 0.413 0.121 22.1 0.166 0.327 16.0 215 1.24 15.8 0.061 0.258 0.036 0.037 0.038 C12.1 C14 C14.1 C14.1.OH C14.2 C14.2.OH C16 C16.0H C16.1 C16.1.OH C16.2 C16.2.OH C18 C18.1 C18.1.OH 4 0.275 0.026 0.028 0.011 0.074 0.011 0.015 0.009 0.020 0.035 0.010 0.013 0.008 0.006 0 004 5 0.394 0.034 0.043 0.016 0.025 0.017 0.062 NA 0.024 0.014 0.012 0.025 0.031 0.034 0.012 0.007 0.060 0.006 0.010 0.008 0.020 0.025 8 0.174 0.024 0.017 0.007 0.006 0.005 0.004 0.004 9 0.228 0.022 0.018 0.007 0.007 0.007 0.054 0.005 0.012 0.005 0.005 0.009 0.014 0.026 0.003 C18.2 C2 C3 C3.OH C3.1 C4 C3.DC..C4.OH. C4.1 C5 C5.M.DC C5.OH..C3.DC.M. C5.1 C5.1.DC 0.026 0.030 0.020 0.077 0.031 0.145 0.034 0.099 0.069 0.141 0.094 4 0.033 2.10 0.278 0.010 0.017 0.110 0.041 0.035 0.016 5 0.017 5.62 0.436 0.029 0.035 0.106 0.058 0.073 0 049 8 0.019 1.66 0.258 0.008 0.012 0.082 0.047 0.021 0.107 0.023 0.023 0.021 0.017 9 0.016 2.21 0.233 0.008 0.014 0.088 0.029 0.024 0.127 0.024 0.024 0.025 0.016 C8 C9 lysoPC.a.C14.0 lysoPC.a.C16.0 lysoPC.a.C16.1 C6..C4.1.DC. C5.DC..C6.OH. C6.1 C7.DC 2.23 0.014 0.018 0.011 0.062 0.016 1 0.022 37 9 2.66

0.209

2.39

32.8

2.19

_	0.050	0.040.0	040 0 026	0 100 0	0.41	1 00	0.4 5	1 07	
5 8	0.052 0.036	0.040 0	.040 0.036	0.192 0.		1.88	24.5 33.7	1.27 3.09	
9	0.036		.015 0.013			2.10	36.0	3.46	
	lysoPC.a.C17.0								C.a.C24.0
1	0.446	9.00	-	8.58	7.27	-	.83	8.25	0.079
4	0.323	7.23		7.22	7.62	1	.64	6.75	0.066
5	0.382	6.6	6	5.39	3.60	0	.97	6.26	0.084
8	0.455	6.9	6	7.31	7.53	2	.35	8.73	0.061
9	0.435	7.2		8.11	6.75		.08	7.82	0.068
	lysoPC.a.C26.0	_	_	_					
1	0.113	0.053		0.108	0.072	0.082	0.438	0.571	2.35
4	0.086	0.04		0.076	0.076	0.076	0.486	0.685	3.33
5	0.118	0.053		0.092	0.072	0.069	0.401	0.513	1.78
8	0.083	0.04		0.124	0.078	0.082	0.424	0.605	2.32
9	0.083 PC.aa.C32.0 PC.	0.03		0.096	0.061	0.064	0.430	0.486	2.05
1	11.4	9.22	0.092	109.0		1.430	0.200	2.38	21.7
4	18.6	13.30	0.079	106.0		1.590	0.190	2.57	20.9
5	13.8	5.03	0.102	83.4		0.709	0.135	1.83	20.5
8	12.1	11.50	0.093	83.6		1.580	0.251	2.16	18.4
9	10.4	11.40	0.082	89.6	55.1	1.390	0.221	1.62	18.3
	PC.aa.C36.2 PC.	.aa.C36.3 PC.aa	a.C36.4 PC	.aa.C36.5	PC.aa.C36.6	PC.aa.C38.0	PC.aa.C38.3	PC.aa.C38.4	PC.aa.C38.5
1	42.4	42.7	120.0	1.86	0.084	1.230	32.1	95.1	16.8
4	48.8	41.2	122.0	1.76		1.160	28.7	92.7	14.3
5	28.5	21.9	98.1	1.70		1.100	23.3	101.0	13.8
8	34.4	41.5	110.0	2.03		1.150	31.3	81.7	14.5
9	32.0	41.8	102.0	1.77		0.902	31.1	75.9	13.6
	PC.aa.C38.6 PC.								
1	41.6 29.9	0.195 0.220	0.074	0.491		5.66 5.06		0.364	0.226 0.223
5	36.2	0.220	0.097	0.433		5.06	22.5	0.427	0.223
8	42.8	0.225	0.099	0.384		5.49	20.6	0.365	0.193
9	37.6	0.181	0.100	0.298		4.88	17.5	0.396	0.216
	PC.aa.C42.2 PC.								
1	0.108	0.272	0.272	0.291		0.027	0.022	1.65	0.371
4	0.119	0.268	0.267	0.254	0.223	0.049	0.023	2.47	0.459
5	0.083	0.206	0.205	0.280	0.095	0.082	0.023	1.72	0.316
8	0.089	0.266	0.237	0.288	0.212	0.028	0.033	1.68	0.335
9	0.086	0.215	0.206	0.223		0.012	0.022	1.53	0.291
	PC.ae.C34.0 PC.								
1	0.880	3.66	2.48	0.813		5.64	1.90	1.17	6.96
4 5	0.964	4.06	3.09	1.020		4.75	2.01	1.35	8.36
8	1.060 1.140	3.28 3.51	1.70	0.722		5.95 5.65	1.47 1.97	0.76 1.25	4.78 7.15
9	0.683	3.20	2.20	0.663		4.79	1.54	1.12	6.43
	PC.ae.C36.5 PC.								
1	4.79	0.474	0.538	2.66		5.51	1.95	0.574	0.575
4	5.97	0.397	0.144	1.97	5.99	5.63	1.97	0.425	0.540
5	4.00	0.430	0.246	1.80	5.45	4.34	1.51	0.430	0.432
8	4.04	0.550	0.559	2.90					0.499
9	3.32	0.442	0.224	2.53					0.555
	PC.ae.C40.3 PC.								
1	0.940	1.76	1.77	1.59		0.316			0.264
4	0.742	1.45	1.62	1.25					0.392
5 8	0.632 0.991	1.10 1.84	1.25 1.53	1.47 1.46		0.355 0.271			0.162 0.333
9	0.737	1.35	1.34	1.40					0.319
	PC.ae.C42.5 PC.								
1	0.888	0.065	0.168	0.536		1.4		.330	2.07
4	0.863	0.069	0.237	0.517				.480	2.97
5	0.513	0.081	0.154	0.178		0.9	87 1.	.480	1.96
8	0.861	0.085	0.183	0.534	0.429	1.5	00 1	.160	2.98
9	0.925	0.069	0.184	0.671	0.460	1.2	30 0	.984	2.21
	SMOHC22.2 S								
1	1.86	0.597	44.9	7.99		0.40 0.29			147 0.337
4	2.84	0.682	52.4	8.61		1.50 0.26			138 0.353
5	1.74	0.478	40.6	5.86		8.34 0.19			111 0.283
8	2.59	0.631	37.9	7.92		9.59 0.19			117 0.227
9	2.07 H1 1 H1 Urea	0.507 N L.Arginine N	37.3	6.65		8.48 0.18			.090 0.268
1		_N L.Arginine_1 NA NA		e_n EDTAC NA	NA	xybulyrale X. NA	o.mydroxybut	yrate Acetate NA NA	
_	1100 0000 P	142	-			1471		1111 1112	-

Δ	2652 2652 5	500.8	16.0) 2	7.1	2.5	12.7		7.2	9.8	
5	2258 2258 1	132.5	13.2	2 5	7.9	2.5	35.2		44.7	20.2	
8	2464 2464 1	182.3	49.8	3 6	3.9	0.0	21.7		20.9	19.5	
9	2725 2725 2	255.8	39.0) 6	4.6	2.7	17.1		37.9	20.0	
	Acetoacetate	e Acetone	Betaine	Carnitine	Choline	Creatine	Dimethyl.sulfone	Ethanol	Formate	Glucose	Glycerol
1	N.F	A NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
4	4.8	3 4.0	13.9	7.7	11.8	14.7	1.3	6.4	14.4	629.5	322.0
5	18.9	18.9	33.9	18.5	27.7	35.4	5.5	13.0	40.0	1618.0	271.6
8	15.4	6.6	35.3	13.0	21.5	25.9	5.4	10.2	23.2	2120.5	406.5
9	22.0	9.3	12.0	14.4	15.4	25.3	3.5	5.1	25.0	1644.2	479.9
	Hypoxanthine	e Isobuty	rate Isop	propanol L	actate Ma	alonate					
1	N.F	A	NA	NA	NA	NA					
4	8.6	5	2.5	4.4	1037.7	7.6					
5	0.0)	6.1	11.2	2199.9	11.7					
8	5.8	3	4.5	4.4	1661.4	11.0					
9	5.6	5	5.9	6.7	2048.5	8.0					
[reached 'ma	ax' / get	Option("n	max.print") omit	ted 1 ro	ws]				